

---

## A Note on Approximate Inverse Iteration

Harry Yserentant

November 13, 2016

**Abstract** Different variants of approximate inverse iteration like the locally optimal block preconditioned conjugate gradient method became in recent years increasingly popular for the solution of the large matrix eigenvalue problems arising from the discretization of selfadjoint elliptic partial differential equations, in particular for the calculation of the minimum eigenvalue. We extend in this little note the classical convergence theory of D'yakonov and Orekhov [Math. Notes 27 (1980)] to the case of operators with an essential spectrum on infinite dimensional Hilbert spaces and allow for arbitrary, sufficiently small perturbations of the solutions of the equation that links the iterates. The note complements the much more elaborate convergence theory of Neymeyr and Knyazev and Neymeyr for the matrix case; see [Knyazev and Neymeyr, SIAM J. Matrix Anal. Appl. 31 (2009)] and the references therein.

**Mathematics Subject Classification (2000)** 65N25 · 65N15 · 65N30

### 1 Introduction

Preconditioned inverse iteration evolved in recent years into a very popular method for the solution of the large matrix eigenvalue problems that arise from the discretization of linear selfadjoint elliptic partial differential equations, in particular in form of the locally optimal (block-)preconditioned conjugate gradient method [2]. The analysis of such methods essentially started with the work of D'yakonov and Orekhov [1] from the early 1980's. In a series of groundbreaking papers, Neymeyr [5, 6, 7] and Knyazev and Neymeyr [3, 4] analyzed these methods in great detail and determined the exact convergence rate of their basic variant. The resulting estimates are short and elegant, but their proof is by no means simple and requires a long, complicated, and tedious analysis. Their generalization to the infinite dimensional case is anything but obvious and necessitates additional considerations [8], in particular in the presence

of an essential spectrum as in the example of the electronic Schrödinger equation, a basic equation of quantum physics and chemistry. Therefore we adapt in this little note the original, comparatively simple and short proof of D'yakonov and Orekhov [1] to this general situation and derive, in the language of quantum mechanics, a variant for the calculation of the ground state energy, the minimum eigenvalue, and an associated eigenfunction. The price to be paid is that the initial approximation of this eigenfunction, from which the iterative process starts, must already possess a Rayleigh quotient below the rest of the spectrum and that the derived error bounds are surely not best possible. They show, however, qualitatively the right behavior, that is, they depend like the best possible bounds for the matrix case only on the minimum eigenvalue and its distance to the rest of the spectrum and on a constant that controls the accuracy of the approximate solutions of the equation that links the iterates. Our presentation is completely based on the weak form of the eigenvalue problem and refers to it only via the assigned bilinear forms.

## 2 Approximate inverse iteration in a general setting

Let  $H$  be a Hilbert space that is equipped with the inner product  $a(u, v)$  inducing the energy norm  $\|u\|$ , under which it is complete, and a further inner product  $(u, v)$  that induces the weaker norm  $\|u\|_0$ . Let the infimum of the Rayleigh quotient

$$\lambda(u) = \frac{a(u, u)}{(u, u)}, \quad u \neq 0 \text{ in } H, \quad (2.1)$$

be an isolated eigenvalue  $\lambda_1 > 0$  of finite multiplicity, which means in particular that the norm  $\|u\|_0$  of an element  $u \in H$  can be estimated by its energy norm  $\|u\|$ . Let  $E_1$  be the corresponding eigenspace, the finite dimensional space of all  $u \in H$  for which

$$a(u, \chi) = \lambda_1(u, \chi), \quad \chi \in H, \quad (2.2)$$

or equivalently  $\lambda(u) = \lambda_1$  holds. Our primary aim is the calculation of this eigenvalue, in quantum mechanics the ground state energy of the system under consideration, and to a lesser degree also of an eigenvector for this eigenvalue.

As  $a(u, \chi_1) = \lambda_1(u, \chi_1)$  for all  $\chi_1 \in E_1$  and as  $\lambda_1 \neq 0$ , the orthogonal complement

$$E_1^\perp = \{u \in H \mid (u, \chi_1) = 0 \text{ for all } \chi_1 \in E_1\} \quad (2.3)$$

of  $E_1$  with respect to the inner product  $(u, v)$  is at the same time the  $a$ -orthogonal complement of this eigenspace. Let  $\lambda_2$  be the infimum of the Rayleigh quotient on  $E_1^\perp$ , itself a point in the spectrum. Since  $\lambda_1$  is an isolated eigenvalue,  $\lambda_2 > \lambda_1$ . In most cases,  $\lambda_2$  will also be an isolated eigenvalue, even in the presence of an essential spectrum as in the example of the electronic Schrödinger equation, but neither this nor any other additional assumption on the structure of the spectrum will enter into our argumentation.

Given an element  $u \in H$  with norm  $\|u\|_0 = 1$  and Rayleigh quotient  $\lambda(u) < \lambda_2$ , in inverse iteration in its original, exact version at first the solution  $w \in H$  of the equation

$$a(w, \chi) = a(u, \chi) - \lambda(u)(u, \chi), \quad \chi \in H, \quad (2.4)$$

is determined, which exists by the Lax-Milgram or the Riesz representation theorem and is unique. The current  $u$  is then replaced by  $u - w$ . Since  $a(u, w) = 0$ ,

$$\|u - w\|^2 = \|u\|^2 + \|w\|^2. \quad (2.5)$$

The new element  $u - w$  is thus different from zero so that  $\lambda(u - w)$  is well defined and the process can be repeated with the normed version of  $u - w$ . The in this way iteratively generated sequence of Rayleigh quotients decreases then monotonously to the eigenvalue  $\lambda_1$  and the iterates  $u$  converge to an eigenvector for this eigenvalue.

This process can hardly be realized when  $H$  is infinite dimensional or of high finite dimension. In the modification considered in this note, the solution  $w$  of equation (2.4) is therefore replaced by an approximation  $v$  for which an error estimate

$$\|v - w\| \leq \eta \|w\| \quad (2.6)$$

holds, where  $\eta < 1$  is a fixed constant that controls the accuracy. By (2.5) and (2.6)

$$\|u - v\| \geq (1 - \eta) \|u - w\|, \quad (2.7)$$

so that also  $u - v \neq 0$  and the whole process can proceed with the new iterate

$$u' = \frac{u - v}{\|u - v\|_0}. \quad (2.8)$$

We do not make any assumption on the origin of  $v$ . It can, for example, be the element of best approximation of  $w$  in an appropriately chosen finite dimensional subspace of  $H$ , an iteratively calculated approximation of this element, or anything else. We will analyze in the next section the convergence properties of this general form of approximate inverse iteration along the lines given by D'yakonov and Orekhov.

### 3 Convergence and error estimates

Starting point of our analysis is as described an element  $u \in H$  of norm  $\|u\|_0 = 1$  with Rayleigh quotient  $\lambda(u) < \lambda_2$ . We assume that  $w$  is the unique solution of equation (2.4),  $v$  an approximation of this  $w$  satisfying (2.6), and  $u'$  the normed version (2.8) of  $u - v$ . For abbreviation, we set  $\lambda = \lambda(u)$  and  $\lambda' = \lambda(u')$ . Moreover, we need the  $a$ -orthogonal projection  $P_1$  of the Hilbert space  $H$  onto the eigenspace  $E_1$  for the eigenvalue  $\lambda_1$ , which is at the same time the orthogonal projection of  $H$  to  $E_1$  with respect to the other inner product  $(u, v)$ , and the with respect to both inner products orthogonal projection  $Q = I - P_1$  of  $H$  onto the orthogonal complement (2.3) of  $E_1$ .

**Lemma 3.1** *The energy norm of  $w$  can be estimated from below as follows:*

$$\|w\|^2 \geq \left( \frac{\lambda_2 - \lambda}{\lambda_2} \right)^2 (\lambda - \lambda_1). \quad (3.1)$$

*Proof* For  $f \in H$ , let  $Gf \in H$  be the solution of the equation

$$a(Gf, \chi) = (f, \chi), \quad \chi \in H.$$

The element  $w = u - \lambda Gu$  is then the solution of the equation (2.4). Thus

$$\|w\| \geq \|Qu - \lambda QGu\|.$$

As  $Qu$  and  $QGu$  are in  $E_1^\perp$  and  $Q$  is orthogonal with respect to both inner products,

$$\|QGu\|^2 = (Qu, QGu) \leq \|Qu\|_0 \|QGu\|_0 \leq \lambda_2^{-1} \|Qu\| \|QGu\|.$$

Therefore  $\|QGu\| \leq \lambda_2^{-1} \|Qu\|$ . As  $1 - \lambda \lambda_2^{-1} > 0$ , this yields

$$\|w\|^2 \geq \left( \frac{\lambda_2 - \lambda}{\lambda_2} \right)^2 \|Qu\|^2.$$

As  $P_1 u$  and  $Qu$  are orthogonal to each other and  $\|u\|_0 = 1$ ,

$$\|Qu\|^2 = \|u\|^2 - \|P_1 u\|^2 = \lambda - \lambda_1 \|P_1 u\|_0^2 \geq \lambda - \lambda_1,$$

from which the estimate (3.1) finally follows.  $\square$

**Lemma 3.2** *The distance of  $\lambda$  and  $\lambda'$  can be estimated from below as*

$$\lambda - \lambda' \geq \frac{\lambda(1 - \eta^2)\|w\|^2}{\lambda + (1 - \eta^2)\|w\|^2}. \quad (3.2)$$

*Proof* As  $(u, u) = 1$ ,  $a(u, u) = \lambda$ , and because  $w$  is a solution of equation (2.4),

$$\lambda - \lambda' = \frac{a(w, w) - a(v - w, v - w) + \lambda(v, v)}{1 - 2(u, v) + (v, v)}.$$

Estimating the denominator with help of the assumption (2.6) on the accuracy of  $v$  from below and the nominator using  $\|u\|_0 = 1$  from above, one obtains the estimate

$$\lambda - \lambda' \geq \frac{(1 - \eta^2)\|w\|^2 + \lambda\|v\|_0^2}{1 + 2\|v\|_0 + \|v\|_0^2}.$$

The right hand side becomes, as a function of the norm  $\|v\|_0$ , minimal if

$$\lambda\|v\|_0 = (1 - \eta^2)\|w\|^2$$

and attains then the value on the right hand side of (3.2).  $\square$

**Theorem 3.1** *Under the given assumptions, and if in particular  $\lambda(u) < \lambda_2$ ,*

$$\lambda(u') - \lambda_1 \leq q(\lambda(u))(\lambda(u) - \lambda_1) \quad (3.3)$$

*holds, where  $q(\lambda)$  is the on the interval  $\lambda_1 \leq \lambda \leq \lambda_2$  strictly increasing function*

$$q(\lambda) = 1 - \frac{(1 - \eta^2)\lambda(\lambda_2 - \lambda)^2}{\lambda_2^2 \lambda + (1 - \eta^2)(\lambda_2 - \lambda)^2(\lambda - \lambda_1)}. \quad (3.4)$$

*Proof* The function  $x \rightarrow \lambda x / (\lambda + x)$  is monotonously increasing. If one inserts the estimate (3.1) into the estimate (3.2), one obtains therefore the lower bound

$$\lambda - \lambda' \geq \frac{(1 - \eta^2) \lambda (\lambda_2 - \lambda)^2 (\lambda - \lambda_1)}{\lambda_2^2 \lambda + (1 - \eta^2) (\lambda_2 - \lambda)^2 (\lambda - \lambda_1)}$$

for the difference  $\lambda - \lambda'$  of the two Rayleigh quotients. If  $\lambda > \lambda_1$ , the representation

$$\lambda' - \lambda_1 = \left(1 - \frac{\lambda - \lambda'}{\lambda - \lambda_1}\right) (\lambda - \lambda_1)$$

of  $\lambda' - \lambda_1$  thus yields the estimate (3.3). The function  $q(\lambda)$  possesses the derivative

$$q'(\lambda) = \frac{(1 - \eta^2) (\lambda_2 - \lambda) ((1 - \eta^2) \lambda_1 (\lambda_2 - \lambda)^3 + 2 \lambda_2^2 \lambda^2)}{(\lambda_2^2 \lambda + (1 - \eta^2) (\lambda_2 - \lambda)^2 (\lambda - \lambda_1))^2}$$

and is therefore strictly increasing on the interval under consideration. If  $\lambda = \lambda_1$  and  $u$  is therefore an eigenvector for the eigenvalue  $\lambda_1$ ,  $w = 0$  and thus also  $v = 0$ . The iteration comes then to a halt, it is  $u' = u$  and  $\lambda' = \lambda_1$ , and (3.3) trivially holds.  $\square$

**Lemma 3.3** *The energy norm of the approximation  $v$  of the solution  $w$  of equation (2.4) can be estimated in terms of the distance of the Rayleigh quotient  $\lambda$  to  $\lambda_1$ :*

$$\|v\|^2 \leq \frac{1 + \eta}{1 - \eta} \frac{\lambda_2}{\lambda_1} (\lambda - \lambda_1). \quad (3.5)$$

*Proof* The estimate from Lemma 3.2 is equivalent to

$$\|w\|^2 \leq \frac{1}{1 - \eta^2} \frac{\lambda}{\lambda'} (\lambda - \lambda').$$

As  $\|v\| \leq (1 + \eta) \|w\|$  and  $\lambda_1 \leq \lambda'$  and  $\lambda \leq \lambda_2$ , the inequality (3.5) follows.  $\square$

If one repeats the process, the Rayleigh quotients approach by (3.3) the eigenvalue  $\lambda_1$ . At the same time, the norm of the assigned vectors  $v$  tends by (3.5) to zero.

**Lemma 3.4** *If already  $\|v\|^2 \leq \lambda_1/4$ , the distance of the normed version  $u'$  of the new vector  $u - v$  and the given normed  $u$  satisfies an estimate*

$$\|u - u'\|^2 \leq c(\lambda_2/\lambda_1, \eta) (\lambda - \lambda_1), \quad (3.6)$$

with a constant depending only on  $\eta$  and the ratio  $\lambda_2/\lambda_1$

*Proof* Because  $u$  has the norm  $\|u\|_0 = 1$ , the energy norm of  $u - u'$  can be written as

$$\|u - u'\| = \frac{\|v - (\|u\|_0 - \|u - v\|_0) u\|}{\|u - v\|_0}.$$

The triangle inequality leads therefore to the estimate

$$\|u - u'\| \leq \frac{\|v\| + \|v\|_0 \|u\|}{1 - \|v\|_0}$$

or, because of  $\|v\|_0^2 \leq \lambda_1^{-1} \|v\|^2 \leq 1/4$  and  $\|u\|^2 = \lambda(u)$ ,  $\lambda(u) \leq \lambda_2$ , to

$$\|u - u'\| \leq 2 \left( 1 + \left( \frac{\lambda_2}{\lambda_1} \right)^{1/2} \right) \|v\|.$$

Estimating the norm of  $v$  by (3.5) in terms of  $\lambda(u) - \lambda_1$ , the proposition follows.  $\square$

If one starts therefore with a normed initial approximation  $u = u_0$  in  $H$  with Rayleigh quotient  $\lambda(u_0) < \lambda_2$  and generates in the manner described a sequence of normed  $u_k$ , the Rayleigh quotients  $\lambda(u_k)$  decrease strictly to the minimum eigenvalue  $\lambda_1$  or become stationary there and the estimate

$$\lambda(u_{k+1}) - \lambda_1 \leq q(\lambda(u_k))(\lambda(u_k) - \lambda_1) \quad (3.7)$$

holds. As  $q(\lambda(u_k)) \leq q(\lambda(u_0))$ ,

$$\lambda(u_k) - \lambda_1 \leq q(\lambda(u_0))^k (\lambda(u_0) - \lambda_1), \quad (3.8)$$

so that the Rayleigh quotients converge because of  $q(\lambda(u_0)) < q(\lambda_2) = 1$  rapidly to their limit. When  $k$  goes to infinity, the error reduction factors  $q(\lambda(u_k))$  fall to

$$q(\lambda_1) = 1 - (1 - \eta^2) \left( \frac{\lambda_2 - \lambda_1}{\lambda_2} \right)^2, \quad (3.9)$$

a value less surprisingly worse than the optimal limit value

$$\left( 1 - (1 - \eta) \frac{\lambda_2 - \lambda_1}{\lambda_2} \right)^2 \quad (3.10)$$

that Knyazev and Neymeyr [3] obtain for the matrix case. For sufficiently large  $k$ , when the norms of the assigned  $v_k$  are already sufficiently small, by Lemma 3.4

$$\|u_k - u_{k+1}\|^2 \leq c(\lambda(u_k) - \lambda_1) \quad (3.11)$$

holds with some constant  $c$  that depends only on  $\eta$  and the ratio  $\lambda_2/\lambda_1$ . In view of the error estimate (3.8) for the Rayleigh quotients, the  $u_k$  thus form a Cauchy sequence in the Hilbert space  $H$ . They converge therefore to a limit  $u^*$  of norm  $\|u^*\|_0 = 1$ .

Our final theorem shows that the distance of an arbitrary normed  $u$  with Rayleigh quotient less than  $\lambda_2$  to its best approximation by an element in the eigenspace  $E_1$  can be bounded in terms of the distance of its Rayleigh quotient to the eigenvalue  $\lambda_1$ .

**Theorem 3.2** *For all  $u$  of norm  $\|u\|_0 = 1$  with Rayleigh quotient  $\lambda(u) < \lambda_2$ ,*

$$\|u - P_1 u\|^2 \leq \left( \frac{\lambda_2 - \lambda_1}{\lambda_2} \right)^{-1} (\lambda(u) - \lambda_1). \quad (3.12)$$

*Proof* Let again  $\lambda = \lambda(u)$  for abbreviation. The proof is based on the relation

$$0 = \|u\|^2 - \lambda \|u\|_0^2 = \|P_1 u\|^2 - \lambda \|P_1 u\|_0^2 + \|Qu\|^2 - \lambda \|Qu\|_0^2.$$

Using  $\|P_1 u\|^2 = \lambda_1 \|P_1 u\|_0^2$ ,  $\|Qu\|^2 \geq \lambda_2 \|Qu\|_0^2$ , and moreover that

$$\|Qu\|_0^2 = 1 - \|P_1 u\|_0^2,$$

one obtains from this relation the lower estimate

$$\|P_1 u\|_0^2 \geq \frac{\lambda_2 - \lambda}{\lambda_2 - \lambda_1}$$

for  $P_1 u$ . Since  $\|u - P_1 u\|^2 = \lambda - \lambda_1 \|P_1 u\|_0^2$ , this proves the estimate (3.12).  $\square$

This shows in particular that  $u^* = P_1 u^*$ , so that the in the course of the iteration generated vectors  $u_k$  converge indeed to an eigenvector for the minimum eigenvalue.

## References

1. D'yakonov, E., Orekhov, M.: Minimization of the computational labor in determining the first eigenvalues of differential operators. *Mat. Zametki* **27**, 795–812 (1980). In Russian, English translation: *Math. Notes* 27 (1980), pp. 382–391
2. Knyazev, A.V.: Toward the optimal preconditioned eigensolver: locally optimal block preconditioned conjugate gradient method. *SIAM J. Sci. Comput.* **23**, 517–541 (2001)
3. Knyazev, A.V., Neymeyr, K.: A geometric theory for preconditioned inverse iteration. III. A short and sharp convergence estimate for generalized eigenvalue problems. *Linear Algebra Appl.* **358**, 95–114 (2003)
4. Knyazev, A.V., Neymeyr, K.: Gradient flow approach to geometric convergence analysis of preconditioned eigensolvers. *SIAM J. Matrix Anal. Appl.* **31**, 621–628 (2009)
5. Neymeyr, K.: A geometric theory for preconditioned inverse iteration. I. Extrema of the Rayleigh quotient. *Linear Algebra Appl.* **322**, 61–85 (2001)
6. Neymeyr, K.: A geometric theory for preconditioned inverse iteration. II. Convergence estimates. *Linear Algebra Appl.* **322**, 87–104 (2001)
7. Neymeyr, K.: A geometric theory for preconditioned inverse iteration. IV. On the fastest convergence cases. *Linear Algebra Appl.* **415**, 114–139 (2006)
8. Rohwedder, T., Schneider, R., Zeiser, A.: Perturbed preconditioned inverse iteration for operator eigenvalue problems with applications to adaptiv wavelet discretization. *Adv. Comput. Math.* **34**, 43–66 (2011)